

Hexamethylphosphoramide
680-31-9 | DTXSID6020694

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 8.83 days

Global applicability domain: Outside

Local applicability domain index: 1.10e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Pentane</div> <div>Measured: 40.7</div> <div>Predicted: 6.52</div>	<div>Image not found</div> <div>n-Hexane</div> <div>Measured: 157</div> <div>Predicted: 7.45</div>	<div>Image not found</div> <div>2,2-Dimethylbutane</div> <div>Measured: 880</div> <div>Predicted: 16.2</div>
<div>Image not found</div> <div>Heptane</div> <div>Measured: 88.3</div> <div>Predicted: 7.54</div>	<div>Image not found</div> <div>Octane</div> <div>Measured: 157</div> <div>Predicted: 8.57</div>	